

New bosonization scheme for spin systems in any dimension

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Abstract

We present a new representation of spin operators in terms of bosonic creation-annihilation operators. This representation allows us to formulate a new field-theoretical description of spin systems which is free of any constraints. The corresponding functional integral representations for thermodynamic quantities are given and the application to investigations of Long Range Order in the system is discussed.

Key words: spin operators, constraints, bosonization

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1 Introduction

There are two sources of motivation to search for bosonic representations of spin systems and systems of truncated oscillators: the first is technical while the second is of principle. Indeed, a general problem of any perturbative investigation of spin systems is the complicated diagram technique which originate from spin-spin commutation relations. On the other hand, for systems with the Hamiltonian formulated in terms of the bosonic or fermionic creation -annihilation operators, the diagram technique is standard and straightforward. That is why we need a bosonic representation for the spin operators to cast the complicated technique into the common form and use the field-theoretical machinery. Another set of problems where the bosonic treatment is vital is when looking for Long Range Order (LRO) in the systems. It is well-known that LRO is reflected in appearance of anomalous averages. It is always very tempting to reformulate the problem in such a way that the anomalous averages become amplitudes of a Bose-condensate of some auxiliary bosons. This was a guidline, for example, in Ref. [1] where constraint-free representations was found for Paulions to predict the Bose-condensation of Frenkel excitons. In this paper we go along a similar line and develop a constraint-free description for arbitrary spin system. To this end we make use the approach developed for truncated oscillators in [2].

We have to note that there are several transformations that express the spin operators in terms of the bosonic or fermionic ones [3, 4]. However, all of them require either the restriction of the bosonic Hilbert space which leads to constraints for the bosonic system or restrict the study to 1D systems. The constraints do not cause any problem unless the systems are treated exactly. Since it is very difficult to get exact results for spin systems, some type of approximations should be used. The most popular approximation scheme is based on the mean field description. At this point drawbacks of the constrained description emerge. Indeed, the mean field approximation does not treat local (on-site) constraints in a proper way. It means that instead of many local constraints only one global constraint appears. All together it leads to the problems of the account of unphysical local fluctuations. This effectively returns us to the local constraints and explains the importance of the constraint-free formulation of the mapping from spin systems to bosonic ones.

Similar to the approach of the sigma-model with Wess-Zumino term [4, 5] we treat the constraint on the number of particles on each site exactly. To do this we use the mapping of the orthogonal sum of identical copies of the lattice spin space of states to the bosonic space of states. In this mapping spin operators are represented in the form of a power series of the bosonic creation and annihilation operators. This compels us to deal with infinite series of different vertices in the diagram technique. The choice of relevant contributions in such series should be dictated as usually by features of the concrete problem.

2 Mapping of spins to bosons without constraint

In this section we will describe the mapping from the system of lattice spins to the auxiliary bosonic system. The goal is to escape the introduction of a constraint. To do this we will embed an infinite number of copies of the finite dimensional space of states in the bosonic space of states and then proceed with the consideration of this new (auxiliary) bosonic space.

To explain this in detail, let us first of all consider one degree of freedom (i.e. a single site). Spin operators obey the following commutation relations (for spin $m/2$):

$$\begin{aligned} S^- S^+ - S^+ S^- &= 2S^z, \quad (S^+)^+ = S^-, \quad (S^+)^{m+1} = (S^-)^{m+1} = 0, \\ S^+ &= S^x + iS^y, \quad S^- = S^x - iS^y. \end{aligned} \quad (1)$$

Operators S^+ , S^- and S^z have the following matrix form in the $m + 1$ -dimensional Hilbert space of states \mathcal{H}_B :

$$\begin{aligned} S^+ &= \sqrt{2} \begin{pmatrix} 0 & 0 & 0 & \dots & 0 & 0 \\ \sqrt{m} & 0 & 0 & \dots & 0 & 0 \\ 0 & \sqrt{2(m-1)} & 0 & \dots & 0 & 0 \\ 0 & 0 & \sqrt{3(m-2)} & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & \dots & \sqrt{m} & 0 \end{pmatrix}, \\ S^- &= (S^+)^{Tr}, \quad S^z = \text{diag} \left(-\frac{m}{2} + k, k = 0, \dots, m \right) \end{aligned}$$

with basis $\{|0\rangle, |1\rangle, \dots, |m\rangle\}$ and the obvious notations.

Now we introduce the infinite orthogonal sum $\mathcal{H}_b = \bigoplus \sum_{n=0}^{\infty} \mathcal{H}_{S,n}$ of such m -dimensional Hilbert spaces $\mathcal{H}_{S,n}$ with basis $\{|0\rangle, |1\rangle, \dots, |m-1\rangle\}, \dots, \{|nm+1\rangle, |nm+2\rangle, \dots, |nm+m\rangle\}, \dots\}$. The extensions of operators S^+ , S^- and S^z in this space have the form:

$$\begin{aligned}\hat{S}^+ &= \text{diag}(S^+, S^+, \dots), & \hat{S}^- &= \text{diag}(S^-, S^-, \dots), \\ \hat{S}^z &= \text{diag}(S^z, S^z, \dots).\end{aligned}$$

It follows that all thermodynamic quantities calculated with operators \hat{S}^+ , \hat{S}^- , \hat{S}^z are exactly the same as those calculated with the original operators S^+ , S^- , S^z . Indeed, for example,

$$\langle \hat{S}^+ \hat{S}^- \rangle \equiv \frac{\text{Sp}(\hat{S}^+ \hat{S}^- e^{-\beta(E-\mu)\hat{S}^+ \hat{S}^-})}{\text{Sp}(e^{-\beta(E-\mu)\hat{S}^+ \hat{S}^-})}$$

coincides with the same expressions but without hats due to the block structure of our operators (we should add that the partition functions differ by an infinite numerical constant which does not affect observable physical quantities). The conclusion is still valid if we start with a lattice of spins and then introduce hats for the operators.

3 Bosonic representation for spin operators

Let us now derive the relations for matrix elements of operators \hat{S}^+ , \hat{S}^- and \hat{S}^z . To do this we will follow the method proposed by Chernyak in Ref. [6] for Paulions. The main point of the method is to use the projection operator on the vacuum state of the auxiliary boson system, i.e on the vector $|0\rangle$. This projection operator \mathcal{P} has the following expression in terms of the bosonic creation and annihilation operators:

$$\mathcal{P} = \sum_{l=0}^{\infty} \frac{(-1)^l}{l!} (b^+)^l b^l \equiv: \exp(-b^+ b) : .$$

We now can use this representation to construct the operators \hat{S}^+ , \hat{S}^- and \hat{S}^z which obey algebra (1). Indeed, it is easy to check from the matrix form that the following relations hold:

$$\begin{aligned}\hat{S}^+ &= \sum_{n=0}^{\infty} \sum_{k=0}^{m-1} (b^+)^{mn+k+1} \mathcal{P} b^{mn+k} \frac{\sqrt{(k+1)(m-k)}}{(mn+k)!\sqrt{mn+k+1}}, & \hat{S}^- &= (\hat{S}^+)^+ \\ \hat{S}^z &= \sum_{n=0}^{\infty} \sum_{k=0}^m (b^+)^{mn+k} \mathcal{P} b^{mn+k} \frac{(-m/2+k)}{(mn+k)!}.\end{aligned}\tag{2}$$

It is obvious that these relations satisfy the algebra (1). For the particular case $m = 2$ our formulae reduce to the formulae originally obtained by Chernyak [6] for the case of paulionic operators.

4 Thermodynamics in functional integral representation

The formulae considered above can be applied to construct the Hamiltonian of the auxiliary bosonic system. Let us start with the following Hamiltonian H_S of spins on a lattice:

$$\begin{aligned} H_S &= \sum_{i \neq k} X_{ik} S_i^x S_k^x + \sum_{i \neq k} Y_{ik} S_i^y S_k^y + \sum_{i \neq k} Z_{ik} S_i^z S_k^z + \\ &+ \sum_i (h_{ix} S_i^x + h_{iy} S_i^y + h_{iz} S_i^z) . \end{aligned}$$

Using operators S^+ , S^- one can cast it in the following form:

$$\begin{aligned} H_S &= \frac{1}{2} \sum_{i \neq k} (X_{ik} + Y_{ik}) S_i^+ S_k^- + \frac{1}{4} \sum_{i \neq k} \left\{ (X_{ik} - Y_{ik}) S_i^+ S_k^+ + h.c. \right\} + \\ &+ \sum_{i \neq k} Z_{ik} S_i^z S_k^z + \frac{1}{2} \sum_i \left\{ (h_{ix} - i h_{iy}) S_i^+ + h.c. \right\} + \sum_i h_{iz} S_i^z . \end{aligned}$$

The corresponding Hamiltonian of the auxiliary bosons based on the relations (2) has the form:

$$\begin{aligned} H &= \frac{1}{2} \sum_{i \neq k} (X_{ik} + Y_{ik}) b_i^+ S_{ik} b_k + \frac{1}{4} \sum_{i \neq k} \left\{ (X_{ik} - Y_{ik}) b_i^+ b_k^+ S_{ik} + h.c. \right\} + \\ &+ \sum_{i \neq k} Z_{ik} \sum_{l,m=0}^{\infty} a(l) a(m) (b_i^+)^l (b_k^+)^m b_i^l b_k^m + \\ &+ \frac{1}{2} \sum_i \left\{ (h_{ix} - i h_{iy}) \sum_{l=0}^{\infty} A(l) (b_i^+)^{l+1} b_i^l + h.c. \right\} + \sum_i h_{iz} \sum_{l=0}^{\infty} a(l) (b_i^+)^l b_i^l . \end{aligned}$$

Here the following notations have been introduced:

$$S_{ik} = \sum_{l,m=0}^{\infty} A(l) A(m) (b_i^+)^l (b_k^+)^m b_i^l b_k^m ,$$

$$A(l) \equiv \sqrt{2} \sum_{k=0}^{\min(m-1,l)} \sum_{n=0}^{\left[\frac{l-k}{m}\right]} \frac{(-1)^{l-mn-k}}{(l-mn-k)!} \frac{\sqrt{(k+1)(m-k)}}{(mn+k)! \sqrt{mn+k+1}} ,$$

$$a(l) \equiv \sum_{k=0}^{\min(m,l)} \sum_{n=0}^{\left[\frac{l-k}{m}\right]} \frac{(-1)^{l-mn-k}}{(l-mn-k)!} \frac{(-m/2+1)}{(mn+k)!} .$$

Using the standard procedure, we can write down the functional integral representation of the partition function and correlators of the auxiliary bosonic system and the original system of truncated oscillators. For example, according to the definition and the formula (2), the following relations arise:

$$Z \equiv Sp(e^{-\beta H}) = \int D b^+(t) D b(t) e^S ,$$

$$\langle S_i^+ S_k^- \rangle = \int D b^+(t) D b(t) \sum_{l,m=0}^{\infty} A(l) A(m) (b_i^+(t))^{l+1} (b_k^+(t))^m b_i^l(t) b_k^{m+1}(t) e^S / Z ,$$

where the action S is defined by the form of the Hamiltonian H :

$$\begin{aligned}
S = & \int_0^\beta dt \left(\sum_i \frac{\partial b_i^+(t)}{\partial t} b_i(t) - \frac{1}{2} \sum_{i \neq k} (X_{ik} + Y_{ik}) b_i^+(t) S_{ik}(t) b_k(t) \right. \\
& - \frac{1}{4} \sum_{i \neq k} \left\{ (X_{ik} - Y_{ik}) b_i^+(t) b_k^+(t) S_{ij}(t) + h.c. \right\} \\
& - \sum_{i \neq k} Z_{ik} \sum_{l,m=0}^{\infty} a(l) a(m) (b_i^+(t))^l (b_k^+(t))^m b_i^l(t) b_k^m(t) \\
& - \frac{1}{2} \sum_i \left\{ (h_{ix} - i h_{iy}) \sum_{l=0}^{\infty} A(l) (b_i^+(t))^{l+1} b_i^l(t) + h.c. \right\} \\
& \left. - \sum_i h_{iz} \sum_{l=0}^{\infty} a(l) (b_i^+(t))^l b_i^l(t) \right).
\end{aligned}$$

All other correlators can be obtained in the same manner and give us the bosonic functional integral representation which is free of constraints and limiting procedures. The functional integral form then allows the simplest approach to the derivation of diagram technique rules which are standard ones for the problems in question. It is tempting to note that this technique is much less complicated and much more straightforward than the spin operator technique and is very natural for the consideration of problems concerning Bose-condensation (Long Range Order) in the system just using the standard Bogoliubov's approach to the subject.

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